

2,2-Bis(bromomethyl)-1,3-propanediol
3296-90-0 | DTXSID9020164

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 2.63e-11 cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 6.33e-01

Confidence level: 8.32e-01

Nearest Neighbors from the Training Set

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Propane, 1,1,3-trimethoxy-

Measured: 1.92e-11

Predicted: 2.33e-11

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3-Methoxybutan-1-ol

Measured: 2.36e-11

Predicted: 2.52e-11

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2-(2-Ethoxyethoxy)ethanol

Measured: 5.72e-11

Predicted: 3.59e-11

Image not found

Diethylene glycol diethyl ether

Measured: 2.68e-11

Predicted: 2.50e-11

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2-Butoxyethanol

Measured: 1.86e-11

Predicted: 2.09e-11